Large-Scale Calculation of Fission Barrier Parameters for 5254 Nuclei with $171 \leq A \leq 330$

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In previous *Theoretical Division Nuclear Weapons Highlights* issues, we have discussed calculations of fission potential-energy surfaces as functions of up to five different nuclear shape coordinates as the system evolves from a ground-state shape to two separated fission fragments. The five shape coordinates we consider beyond the second minimum in the fission barrier (fission isomer) are elongation, neck radius, spheroidal deformations of the emerging left and right fragments, and left-right mass asymmetry. For less deformed shapes between the spherical shape and the second minimum in the barrier we consider three shape coordinates in the Nilsson perturbed-spheroid ε parameterization: ε_2 (quadrupole), ε_4 (hexadecapole), and γ (axial asymmetry). Important parameters of the calculated nuclear potential-energy surface, such as the local minima, saddle points between all pairs of minima, valleys as functions of elongation, and the height of the ridges that separate the valleys are extracted by similar immersion techniques to those used in geography. Some illustrative results for a few nuclei have been presented in *Nuclear Weapons Highlights* reports in previous years.

This year we have used our models to undertake production calculations so that we obtain detailed descriptions of the fission potential-energy for a large number of nuclei. Specifically we calculated 5-D potential energy surfaces for 5254 nuclei between the proton and neutron drip lines from A = 171 to A = 330. For each of these nuclei the energy is calculated for 5,009,325 different nuclear shapes. In addition we studied the effect of triaxiality at the first peak in the barrier by calculating 3-D potential-energy surfaces for these same nuclei in the ε parameterization. We have developed highly automated scripts that use our immersion codes to extract relevant barrier structure parameters from the calculated potential-energy surfaces. At this stage we have extracted the heights of the first and second barrier peaks and the fission-isomeric state for all 5254 nuclei.

Figure 1 shows a comparison between calculated and experimental barrier parameters for a sequence of uranium nuclei. The experimental data are from a review by Madland [1]. Sometimes the results of several experiments are plotted for the same isotope. We have made such comparisons for isotope chains of all elements from Th to Es (Z = 90 to Z = 99). Such detailed knowledge about the barrier structure and other nuclear structure properties are necessary to model (n,f), (n,2n), and many other cross sections. The potential-energy calculations took 30000 CPU hours and the subsequent analysis 20000 CPU hours (so far) on the T-16 cluster "nuclei."

To model many astrophysical scenarios; for example to model the end of the rapid-neutron-capture process (r-process) in which many heavy elements are formed in stars, it is necessary to know fission-barrier heights of a large number of nuclei. When a neutron is captured in the r-process it is energetically possible for the nucleus to fission if the neutron binding energy of the compound system is larger than the fission-barrier height. We display in Fig. 2 the difference between the calculated fission-barrier height and the one-neutron separation energy. When this quantity is negative it is energetically possible for the nucleus to fission.

The duration of the large neutron flux that powers the r-process is thought to be of the order of 1 s. Thermonuclear explosions also generate large fluxes of neutrons, but these are of shorter duration, and neutron capture in this environment is therefore referred to as prompt neutron capture. However, this process can be thought of as an approximation to the r-process on earth [2], at least over a limited range of nuclei. Several nuclear weapons tests between 1952 and 1969 involved studies of the prompt capture process. In Fig. 2, we have indicated where capture chains starting with ^{232}Th, ^{238}U, and ^{242}Pu terminate [2]. We note that the U and Pu chains end very near the dark green area, where nuclei would fission immediately upon neutron capture. Thus, our results are very consistent with the experimental observations, and a very encouraging sign that our models produce reliable fission-barrier parameters far from stability. Consequently, another exciting application is to use our calculated database in modeling the end of the r-process, which runs far from stability in regions of experimentally inaccessible nuclei where the neutron separation energy is 1–2 MeV or so. The Th decay chain does not reach the dark green area. However, it was observed [2] that this capture chain is severely blocked at A = 242 and A = 244 where the neutron capture cross section becomes very small. A more detailed interpretation of the observations on these capture chains requires more elaborate calculations of the reaction paths using realistic neutron spectra, which are not all thermal.

In the near future we plan to configure our immersion codes to establish when the calculated potential-energy surfaces exhibit more than one fission mode, the character (mass symmetric division or mass asymmetric division) of the different modes, and the threshold saddle-point energies for these modes.

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[1] D.G. Madland, Los Alamos National Laboratory, personal communication, 2000.
[2] S.A. Becker, *Carnegie Observatories Astrophysics Series*, Vol. 4, A. McWilliam and M. Rauch, Eds. (Pasadena: Carnegie Observatories, http://www.ociw.edu/ociw/symposia/series/symposium4/proceedings.html).

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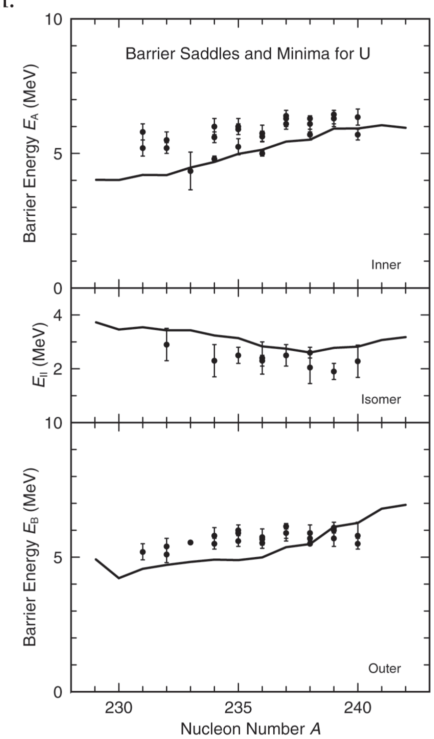

Fig. 1.
Calculated height of the first E_A and second E_B peak in the fission-barrier and calculated energy E_{II} of the fission isomer for U isotopes, compared to experimental data where available. The calculated energies are all relative to the calculated energy of the ground-state minimum.

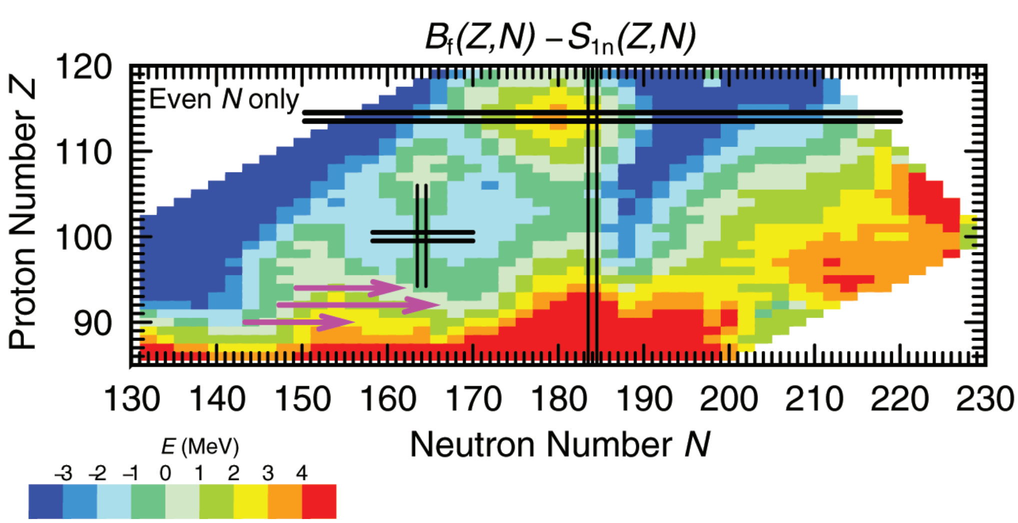

Fig. 2.
Difference between calculated fission-barrier height and neutron separation energy. When this quantity becomes negative (dark green area) fission is energetically possible. We indicate in the figure the beginning and ending of these capture chains observed in weapons tests [2]. Two of the chains (U and Pu) end next to the dark green area where fission becomes energetically possible.